

FIG. 1(a)

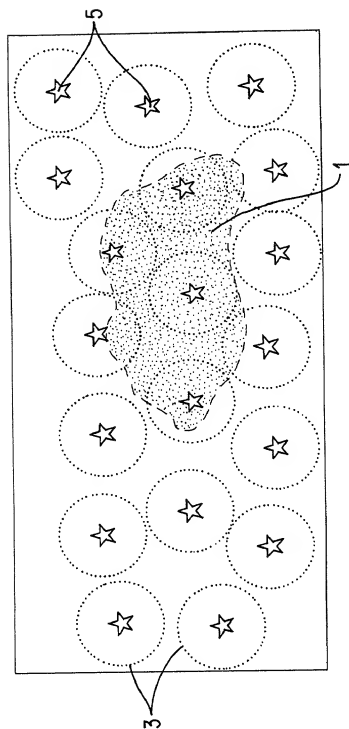


FIG. 1(b)

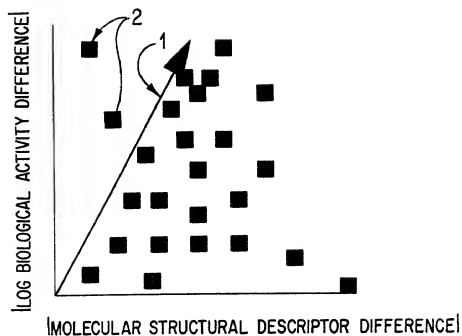


FIG. 2

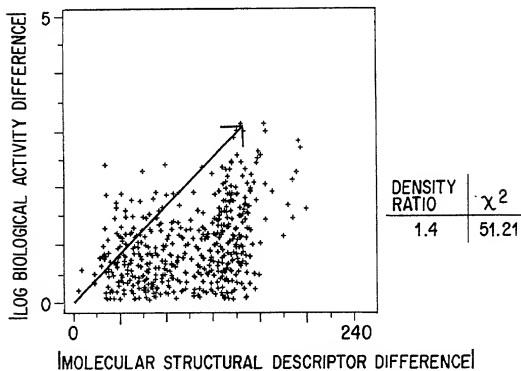
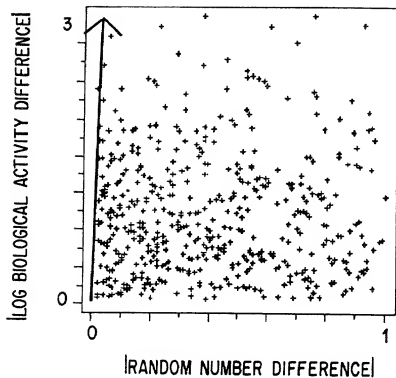
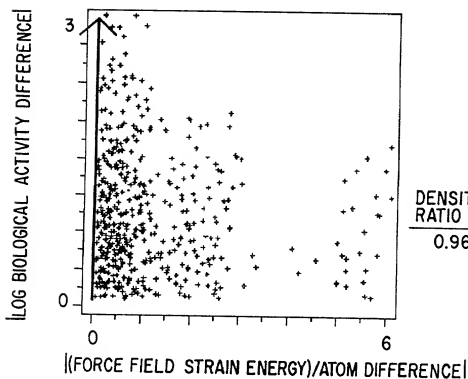


FIG. 3



DENSITY RATIO	χ^2
1.00	0.00

FIG. 4



DENSITY RATIO	χ^2
0.96	0.46

FIG. 5

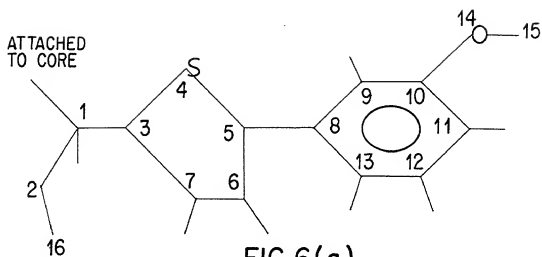


FIG. 6(a)

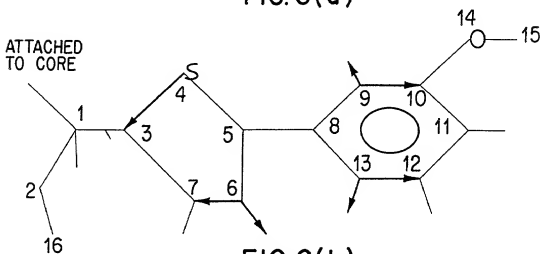


FIG. 6(b)

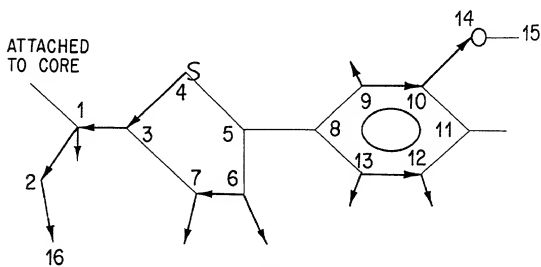


FIG. 6(c)

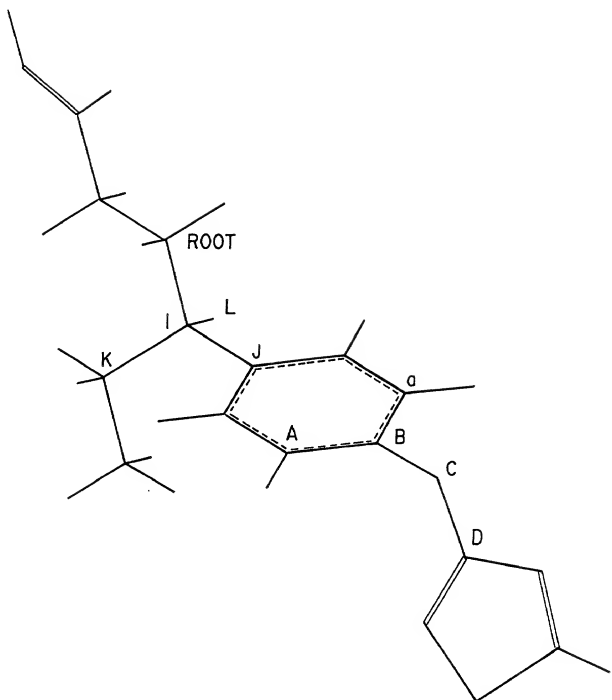


FIG. 6(d)

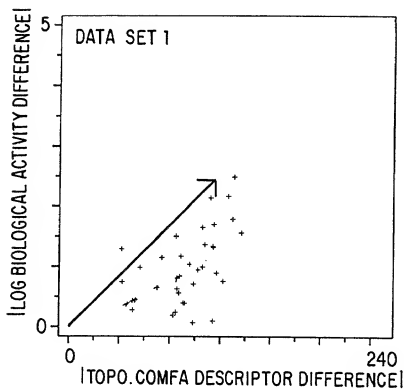


FIG.7(a)

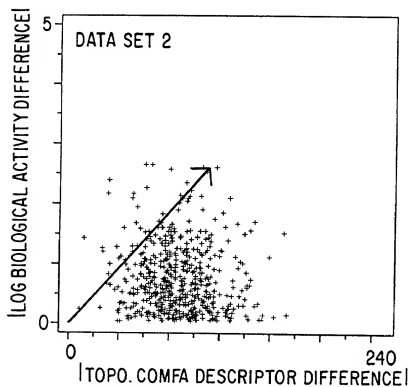


FIG.7(b)

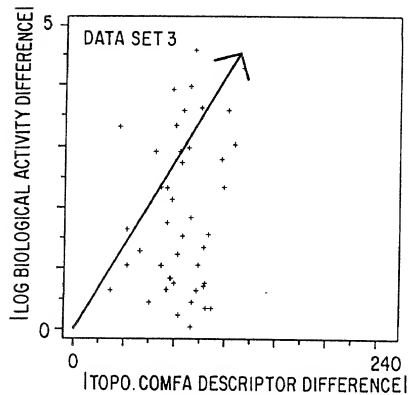


FIG. 7(c)

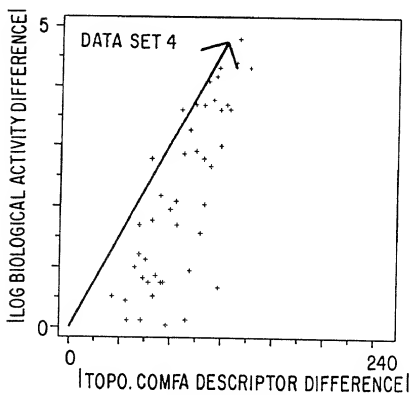


FIG. 7(d)

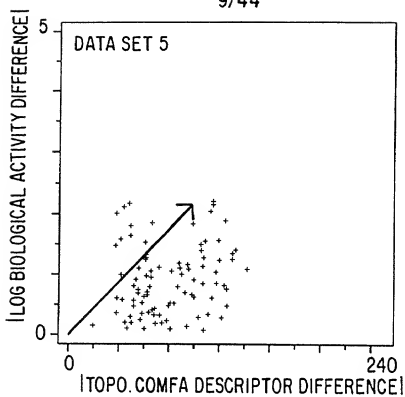


FIG.7(e)

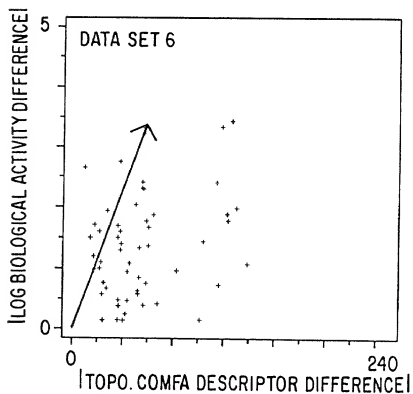


FIG.7(f)

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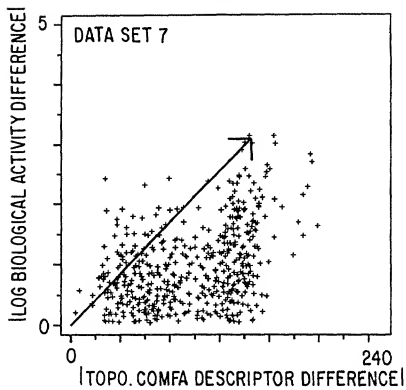


FIG.7(g)

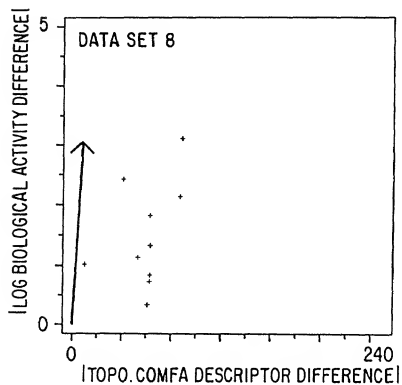


FIG.7(h)

105250*24599860

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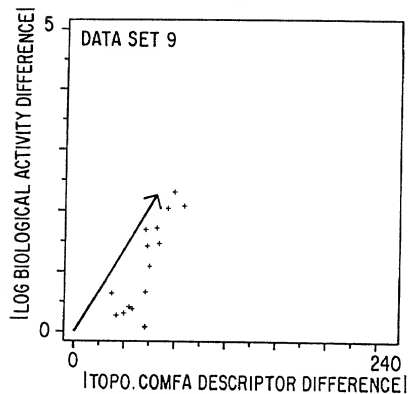


FIG.7(i)

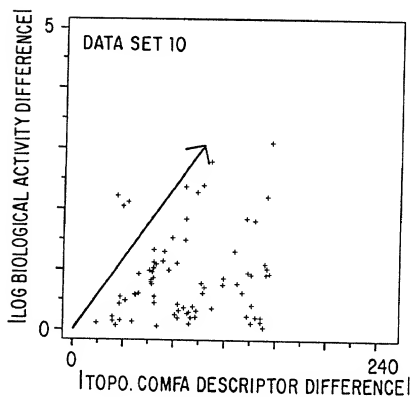


FIG.7(j)

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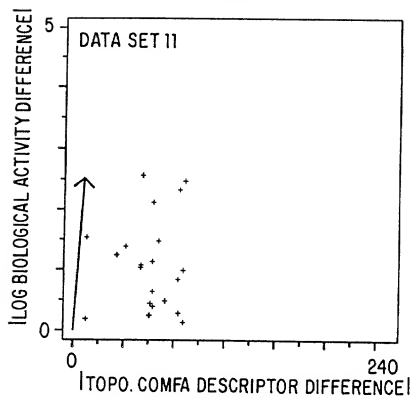


FIG.7(k)

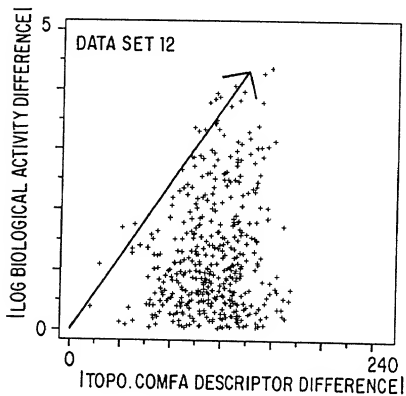


FIG.7(l)

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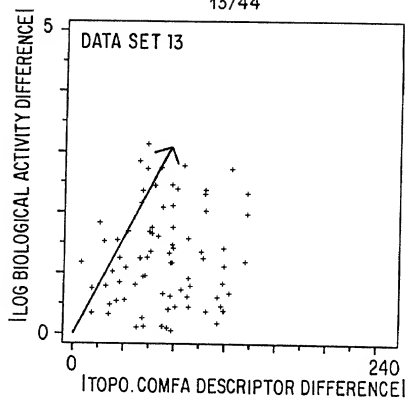


FIG.7(m)

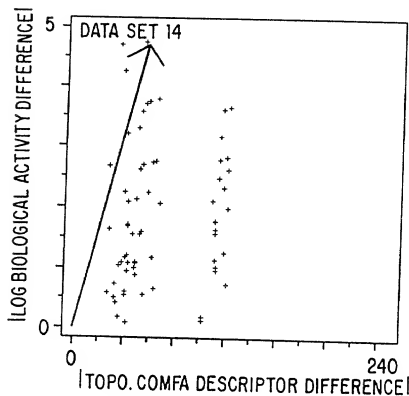


FIG.7(n)

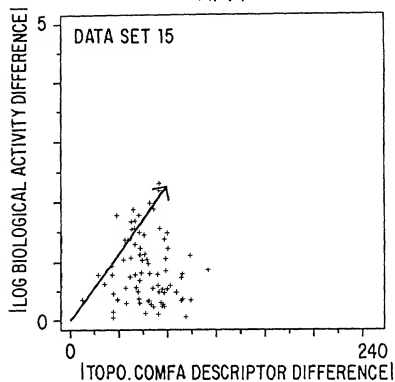


FIG.7(o)

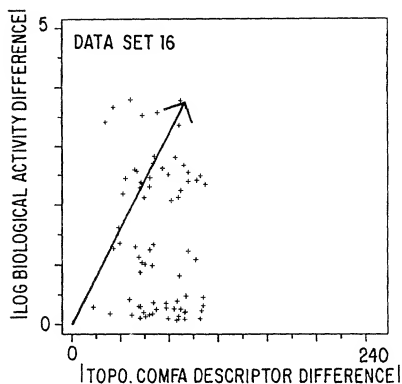


FIG.7(p)

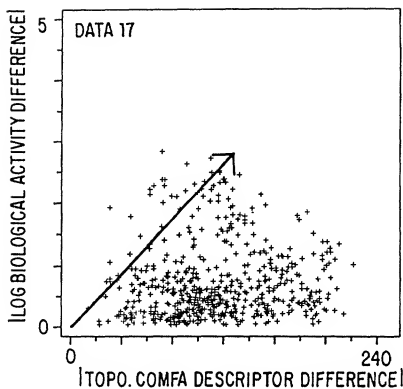


FIG.7(q)

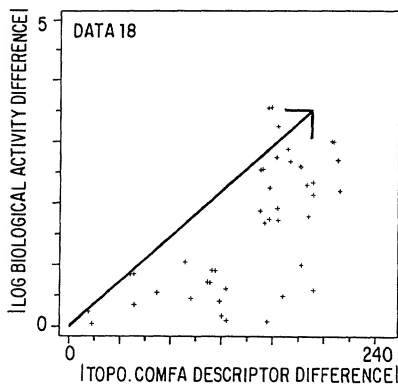


FIG.7(r)

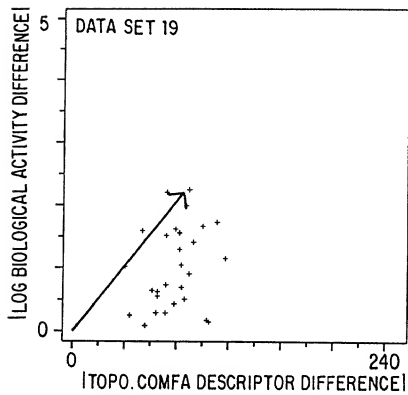


FIG. 7(s)

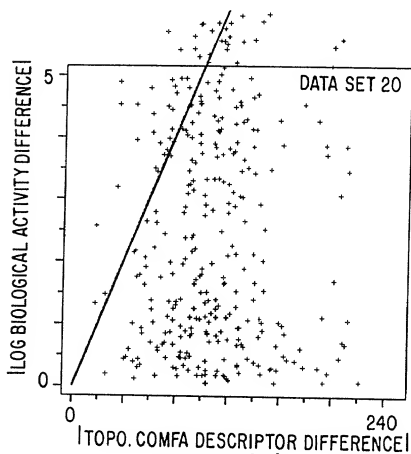


FIG. 7(†)

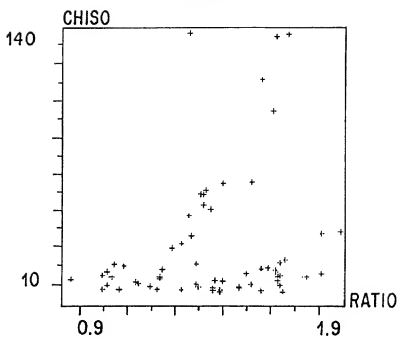


FIG. 8(a)

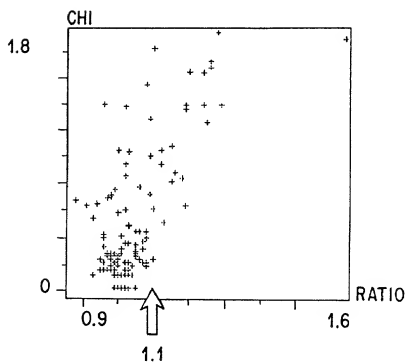


FIG. 8(b)

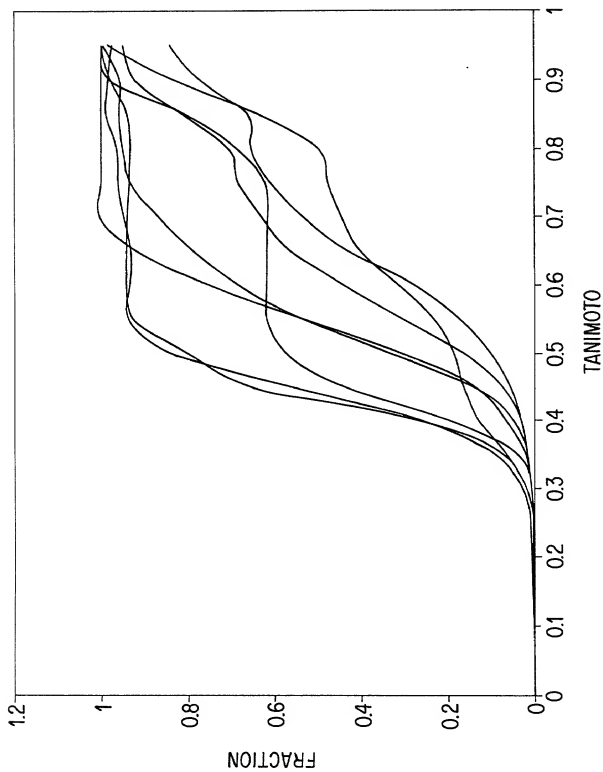


FIG. 9(a)

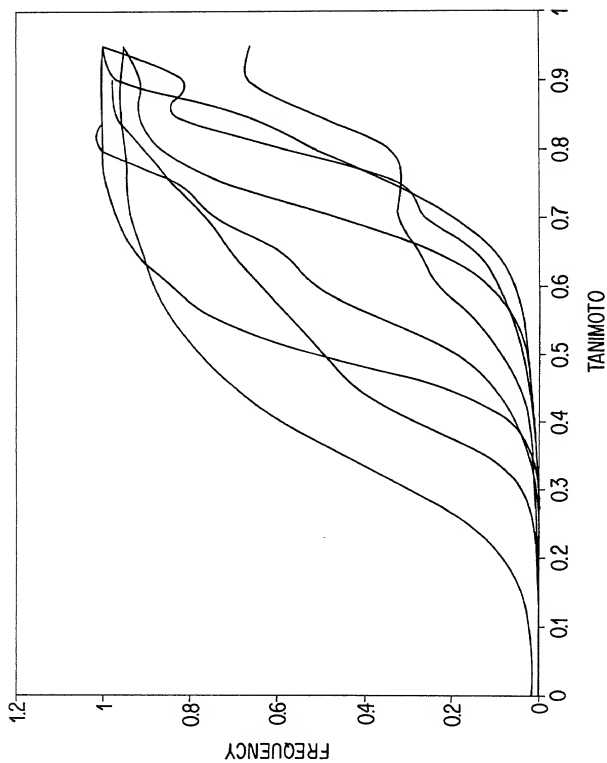


FIG. 9(b)

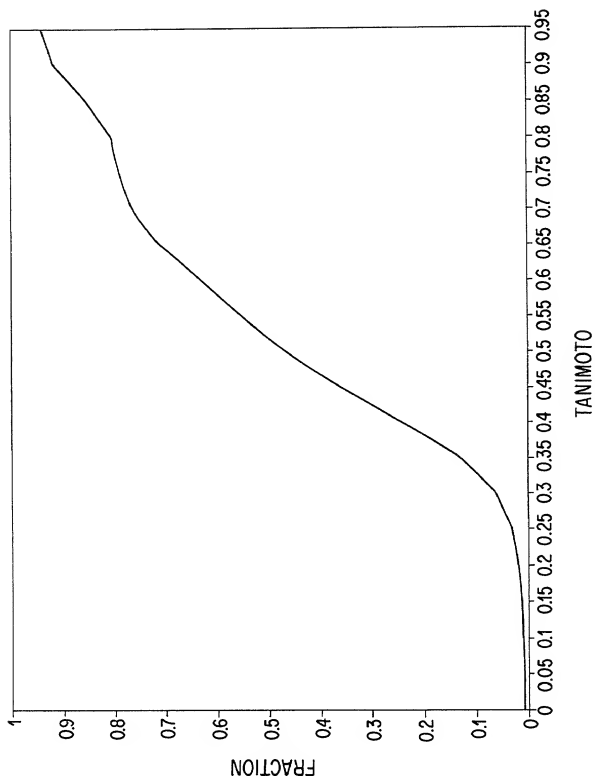


FIG. 9(c)

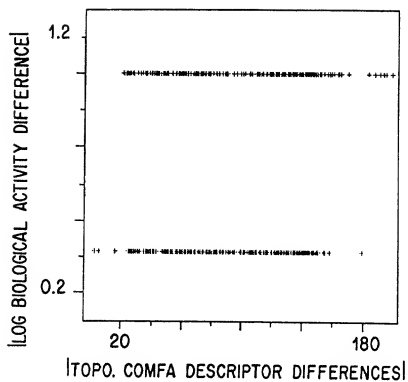


FIG.10(a)

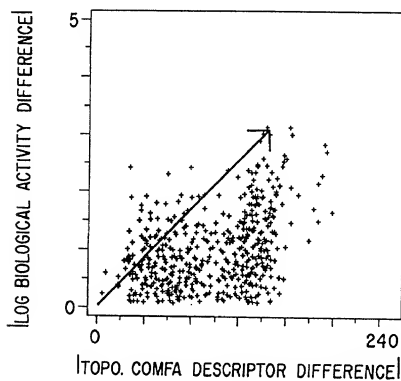


FIG.10(b)

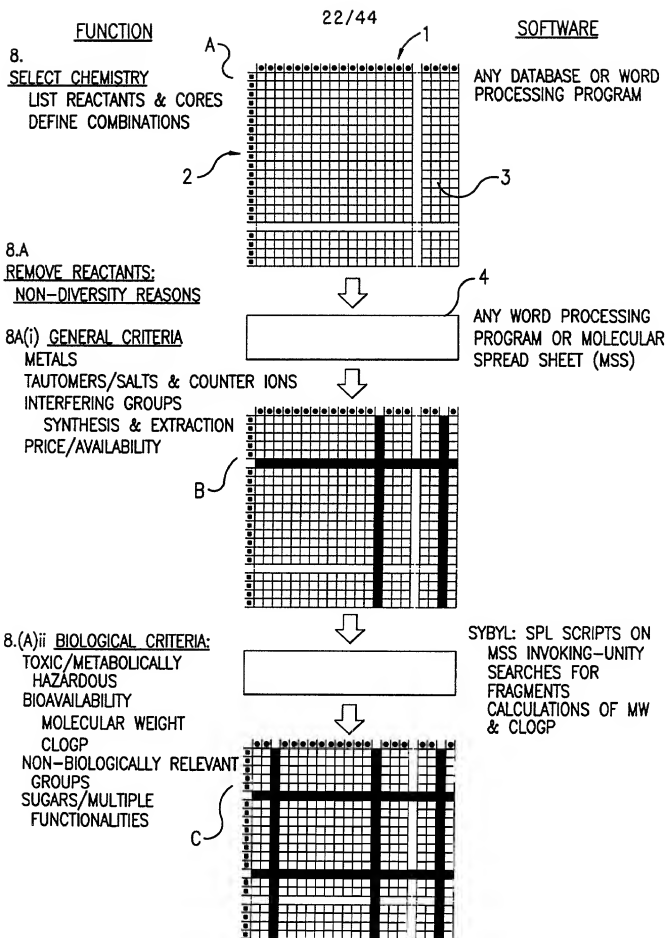


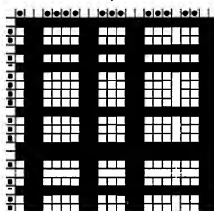
FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION
 TOPOMERIC CONFORMER
 ALIGNMENT
 CoMFA FIELD GENERATION:
 HYDROGEN BOND FIELD
 GENERATION
 ROTATABLE BOND FIELD
 ATTENUATION
 CALCULATE FIELD
 DIFFERENCES
 CLUSTER
 REACTANT SELECTION FROM
 EACH CLUSTER

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SYBYL: SELECTOR &
 CONCORD 3.2.1
 SPECIALIZED SOFTWARE:
 APPENDIX "A"
 (SYBYL: CoMFA
 STERIC & MSS)

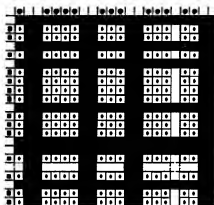
SYBYL: HIERCHICAL
 CLUSTER - MSS
 SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS



E

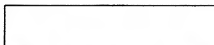


SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:
NON-DIVERSITY REASONS

GENERAL CRITERIA:



SYBYL: SPL SCRIPTS
 ON MSS

F

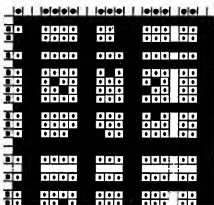


FIG.11(b)

0086547.052501

BIOLOGICAL CRITERIA:

G

SYBYL: SPL SCRIPTS ON
MSS INVOKING -
UNITY SEARCHES FOR
FRAGMENTS
CALCULATIONS OF MW
& CLOGP

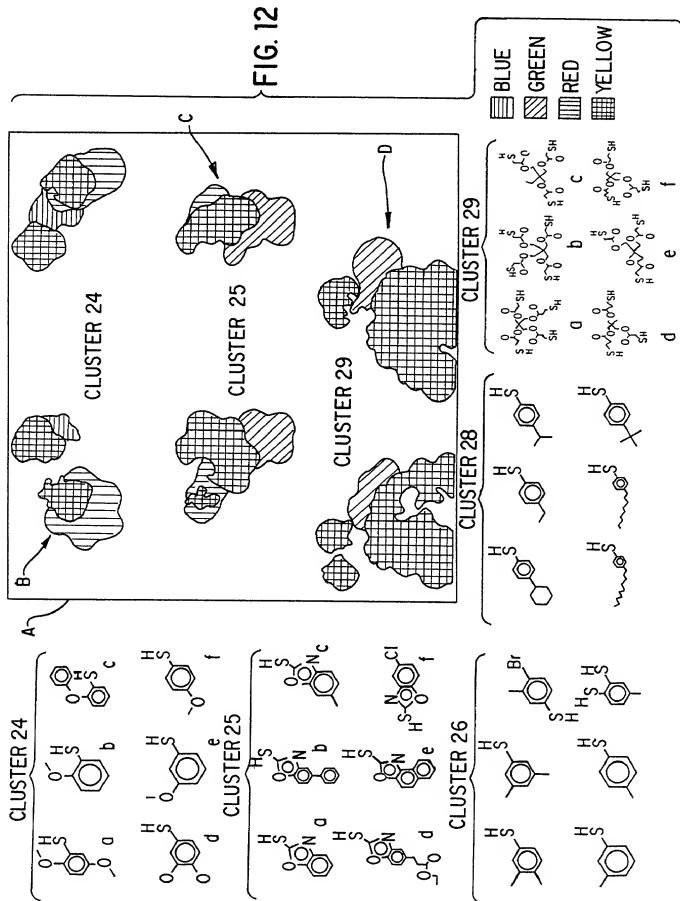
REMOVE NON-DIVERSE
PRODUCTS:

GENERATE TANIMOTO
2D FINGERPRINTS
SAMPLE PRODUCTS:
EXCLUDE TAN > 0.85

H

UNITY

FIG. 11(c)



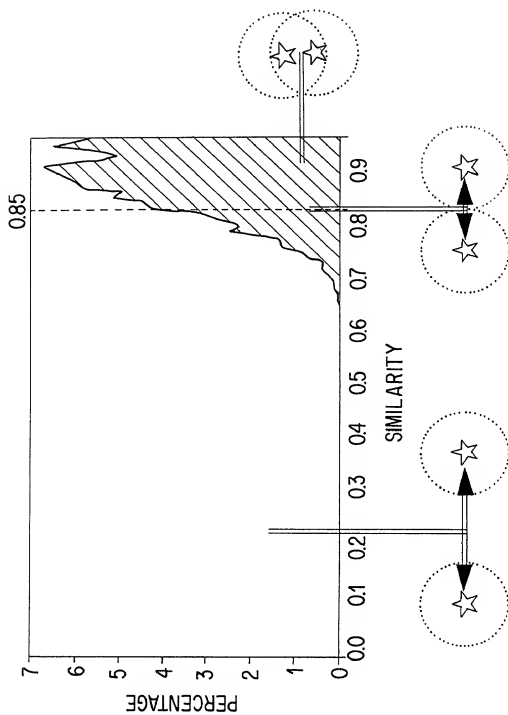


FIG. 13

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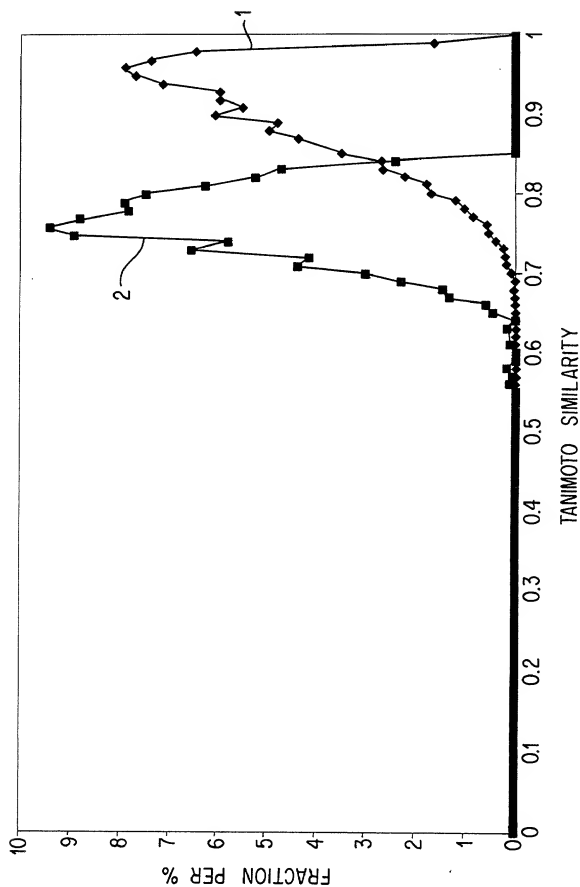


FIG. 14

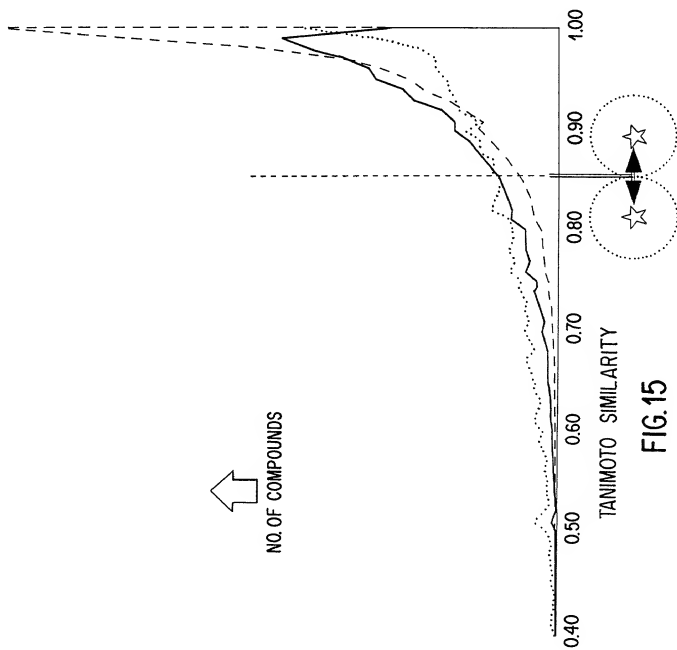


FIG. 15

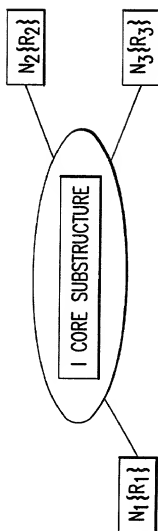


FIG.16

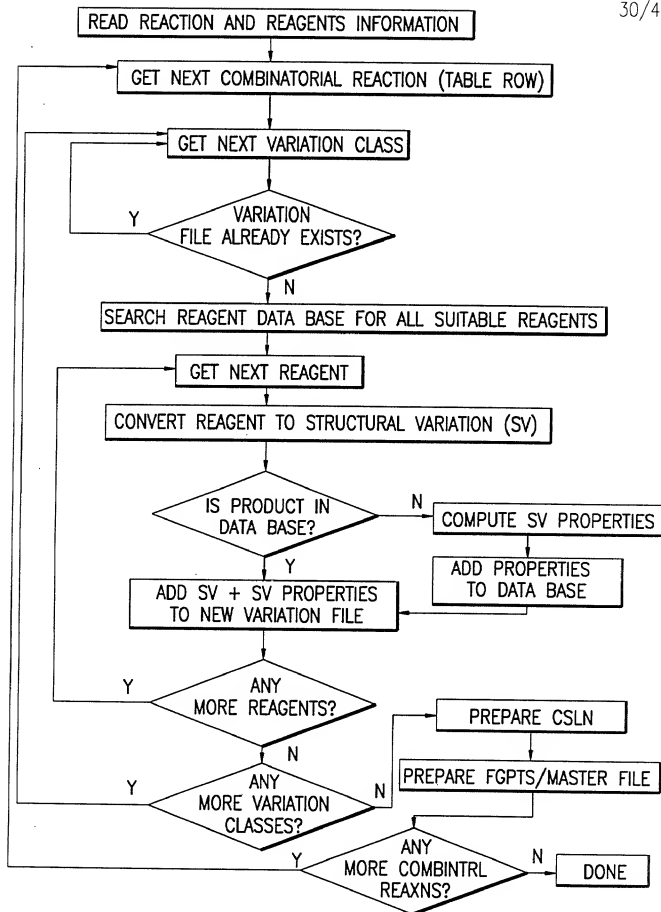


FIG.17

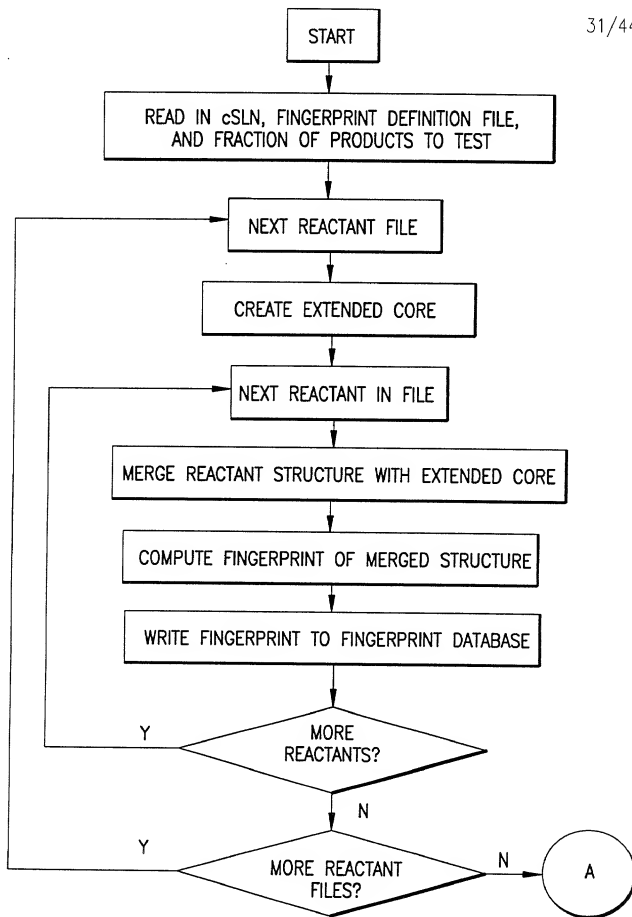


FIG.18

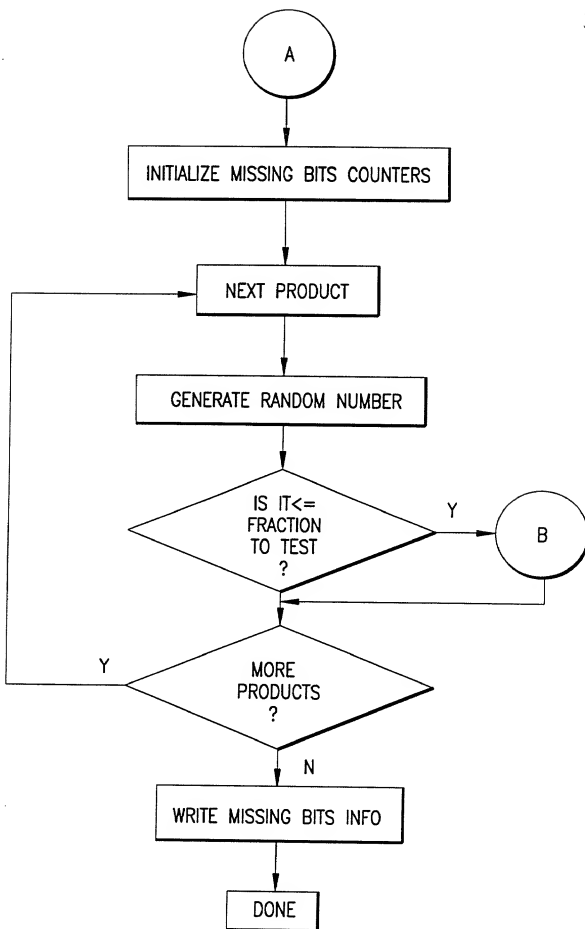


FIG.19

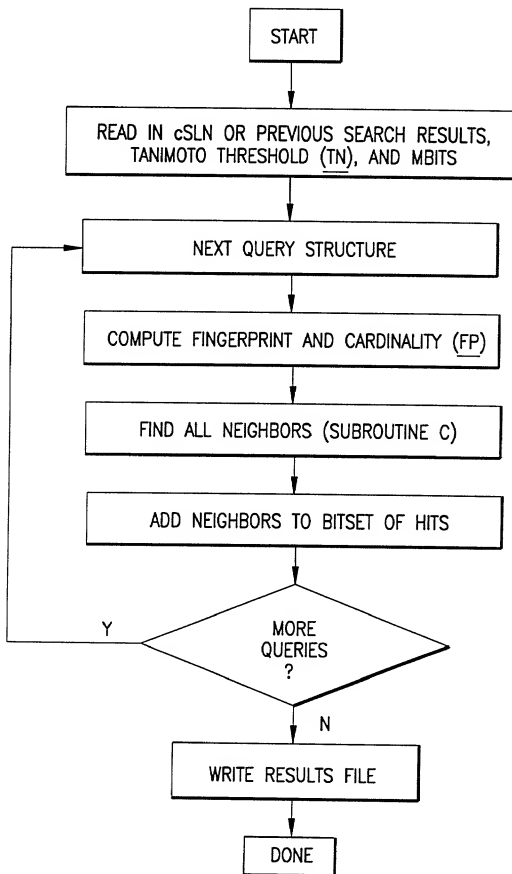
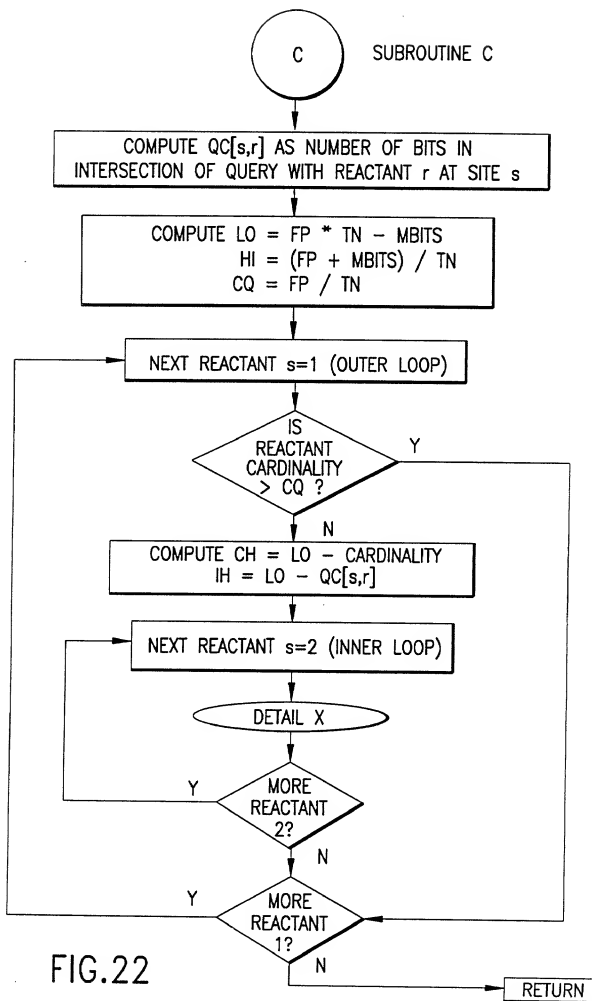


FIG.21



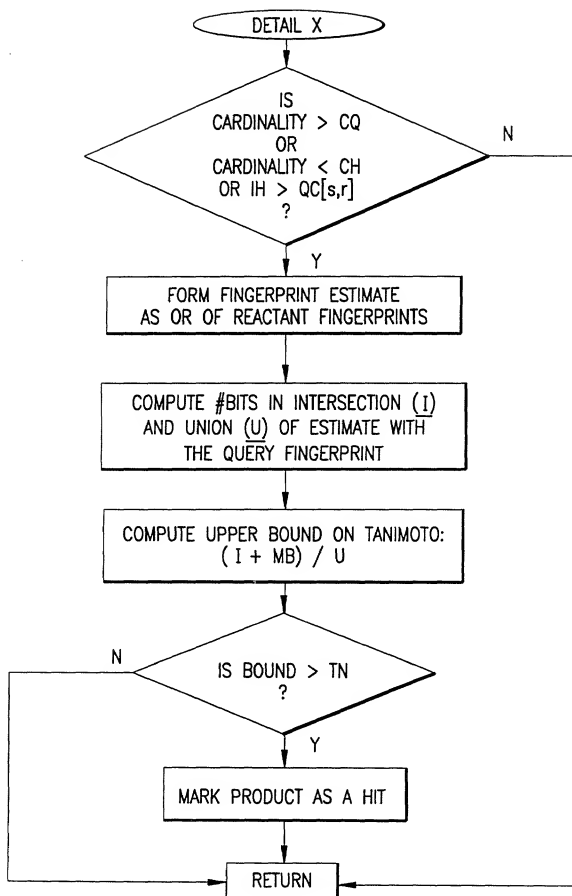


FIG.23

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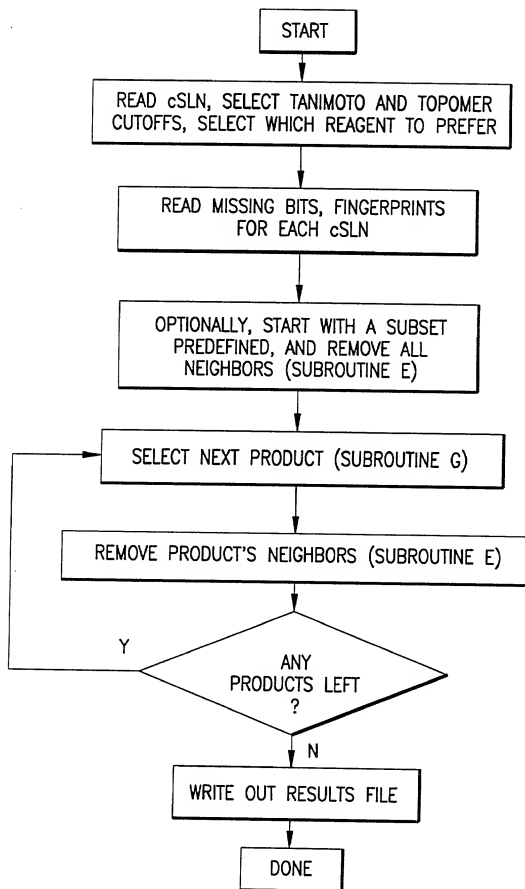


FIG.24

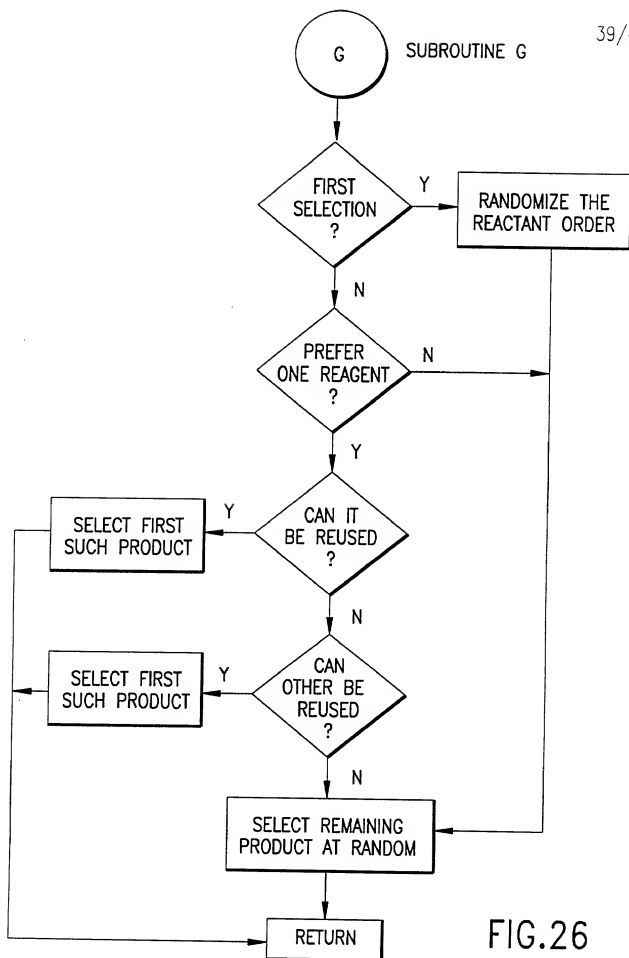


FIG.26

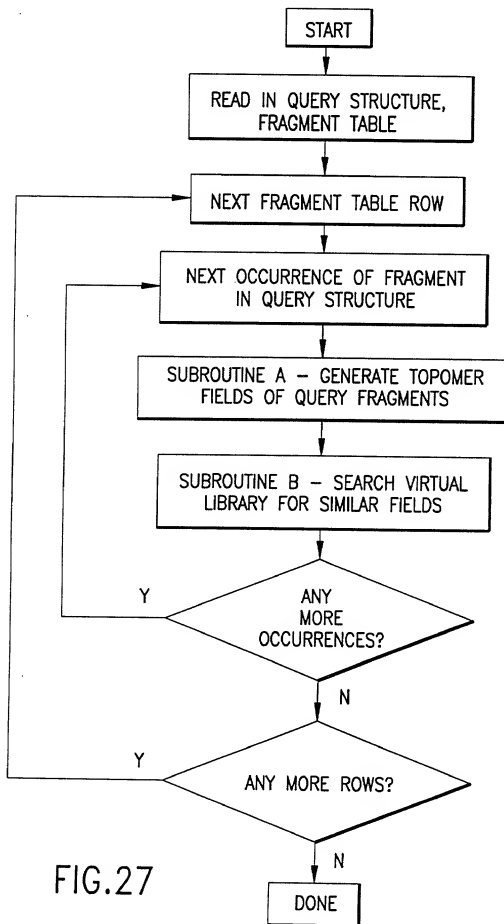


FIG.27

SUBROUTINE A

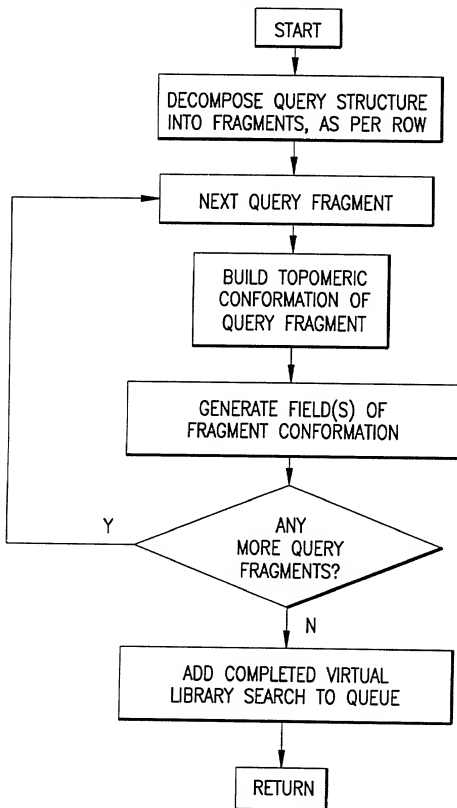


FIG.28

SUBROUTINE B

START

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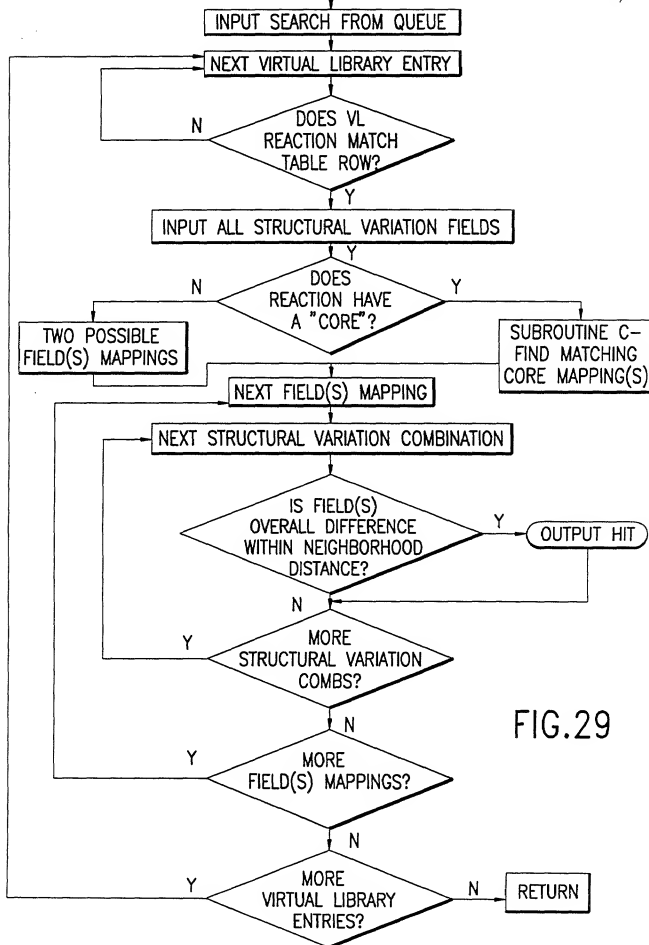


FIG.29

105250-4499860

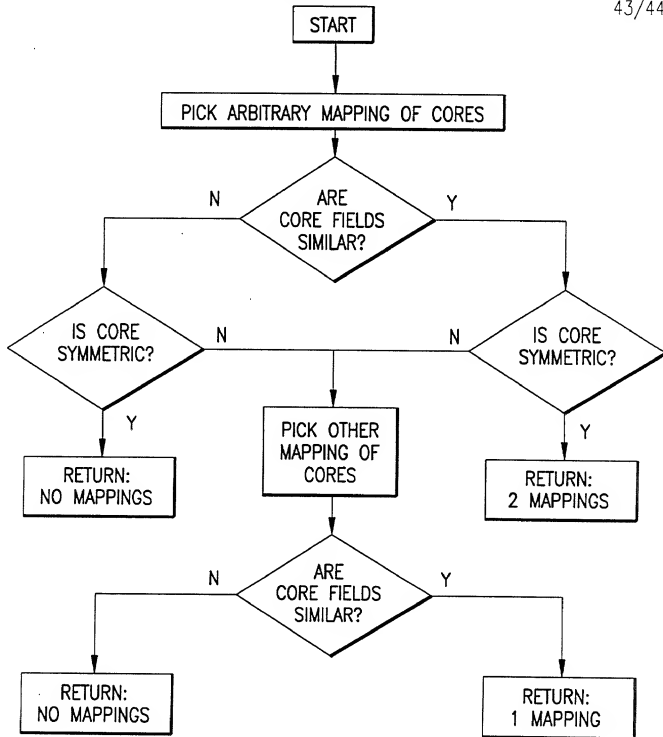


FIG.30

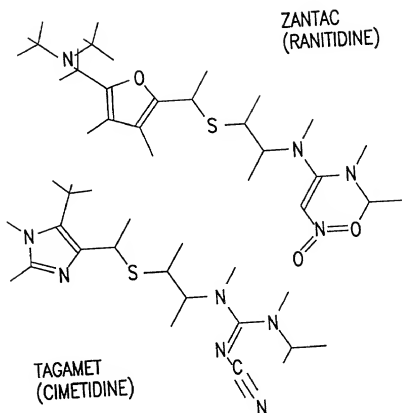


FIG.31